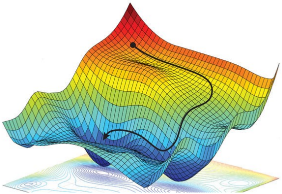
Introduction to Machine Learning

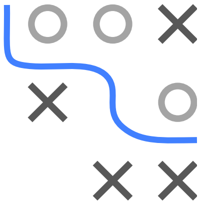
Risk Minimizers



Learning goals

- Bayes optimal model (also: risk minimizer, population minimizer)
- Bayes risk
- Bayes regret, estimation and approximation error
- Optimal constant model
- Consistent learners

EMPIRICAL RISK MINIMIZATION



Very often, in ML, we minimize the empirical risk

$$\mathcal{R}_{\text{emp}}(f) = \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right)$$

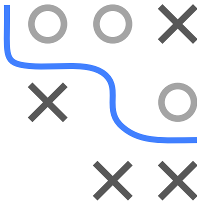
- each observation $\left(\mathbf{x}^{(i)}, y^{(i)}\right) \in \mathcal{X} \times \mathcal{Y}$, so from feature and target space
- $f_{\mathcal{H}} : \mathcal{X} \to \mathbb{R}^g$, f is a model from hypothesis space $\mathcal{H}$; maps a feature vector to output score; sometimes or often we omit $\mathcal{H}$ in the index
- $L : (\mathcal{Y} \times \mathbb{R}^g) \to \mathbb{R}$ is loss;
  $L(y, f)$ measures distance between label and prediction
- We assume that $(\mathbf{x}, y) \sim \mathbb{P}_{xy}$ and $\left(\mathbf{x}^{(i)}, y^{(i)}\right) \overset{\text{i.i.d.}}{\sim} \mathbb{P}_{xy}$
  $\mathbb{P}_{xy}$ is the distribution of the data generating process (DGP)

Let's define (and minimize) loss in expectation, the theoretical risk:

$$\mathcal{R}(f) := \mathbb{E}_{xy}[L(y, f(\mathbf{x}))] = \int L(y, f(\mathbf{x}))\, d\mathbb{P}_{xy}$$

OPTIMAL CONSTANTS FOR A LOSS

- Let's assume some RV $Z \in \mathcal{Y}$ for a label
- Z not Y, because we want to fiddle with its distribution
- Assume Z has distribution Q, so $Z \sim Q$
- We can now consider $\arg\min_c \mathbb{E}_{Z \sim Q}[L(Z, c)]$
  so the score-constant which loss-minimally approximates Z



We will consider 3 cases for Q

- $Q = P_Y$, simply our labels and their marginal distribution in $\mathbb{P}_{xy}$
- $Q = P_{Y|X=x}$, conditional label distribution at point $X = x$
- $Q = P_n$, the empirical product distribution for data $y_1, \ldots, y_n$

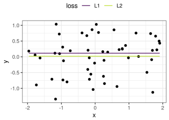
If we can solve $\arg\min_c \mathbb{E}_{Z \sim Q}[L(Z, c)]$ for any Q, we will get multiple useful results!

OPTIMAL CONSTANT MODEL

- We would like a loss optimal, constant baseline predictor
- A "featureless" ML model, which always predicts the same value
- Can use it as baseline in experiments, if we don't beat this with more complex model, that model is useless
- Will also be useful as component in algorithms and derivations

$$f_c^* = \underset{c \in \mathbb{R}}{\arg\min}\, \mathbb{E}_{xy}\left[L(y, c)\right] = \underset{c \in \mathbb{R}}{\arg\min}\, \mathbb{E}_{y}\left[L(y, c)\right]$$

and
$f(\mathbf{x}) = \theta = c$ that optimizes the empirical risk $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ is denoted as as $\hat{f}_c = \arg\min_{c \in \mathbb{R}} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$.



OPTIMAL CONSTANT MODEL

- Let's start with the simplest case, L2 loss
- And we want to find and optimal constant model for

$$\arg\min \mathbb{E}[L(Z, c)] =$$

$$\arg\min \mathbb{E}[(Z - c)^2] =$$

$$\arg\min \mathbb{E}[Z^2] - 2cE[Z] + c^2 =$$

$$E[Z]$$

- Using $Q = P_Y$, this means that, given we know the label distribution, the best constant is $c = E[Y]$.

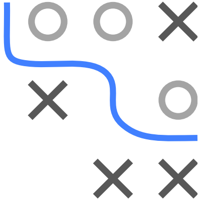
OPTIMAL CONSTANT MODEL

- If we only have data $y_1, \ldots y_n$

  $$\arg\min \mathbb{E}_{Z \sim P_n}[(Z - c)^2] = \mathbb{E}_{Z \sim P_n}[Z] = \frac{1}{n} \sum_{i=1}^{n} y^{(i)} = \bar{y}$$

- And we want to find and optimal constant model for

RISK MINIMIZER

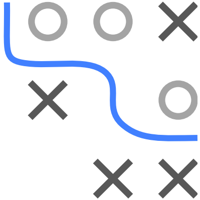


Let us assume we are in an "ideal world":

- The hypothesis space $\mathcal{H}$ is unrestricted. We can choose any $f : \mathcal{X} \rightarrow \mathbb{R}^g$.
- We also assume an ideal optimizer; the risk minimization can always be solved perfectly and efficiently.
- We know $\mathbb{P}_{xy}$.

How should f be chosen?

RISK MINIMIZER



The f with minimal risk across all (measurable) functions is called the **risk minimizer**, **population minimizer** or **Bayes optimal model**.

$$\begin{aligned} f^* &= \mathop{\arg\min}_{f:\mathcal{X}\to\mathbb{R}^g} \mathcal{R}_L(f) = \mathop{\arg\min}_{f:\mathcal{X}\to\mathbb{R}^g} \mathbb{E}_{xy}\left[L\left(y, f(\mathbf{x})\right)\right] \\ &= \mathop{\arg\min}_{f:\mathcal{X}\to\mathbb{R}^g} \int L\left(y, f(\mathbf{x})\right) \mathrm{d}\mathbb{P}_{xy}. \end{aligned}$$

The resulting risk is called **Bayes risk**: $\mathcal{R}_L^* = \mathcal{R}_L(f^*)$

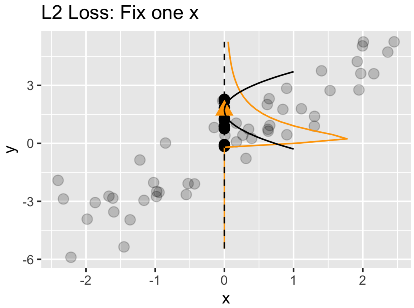
OPTIMAL POINT-WISE PREDICTIONS

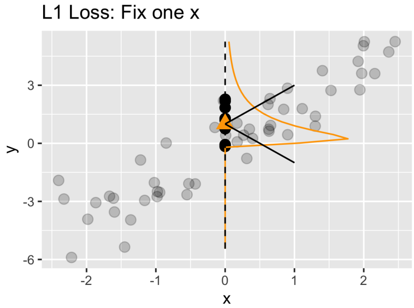
To derive the risk minimizer, observe that by law of total expectation

$$\mathcal{R}_L(f) = \mathbb{E}_{xy}\left[L\left(y, f(\mathbf{x})\right)\right] = \mathbb{E}_x\left[\mathbb{E}_{y|x}\left[L\left(y, f(\mathbf{x})\right) \mid \mathbf{x} = \mathbf{x}\right]\right].$$

- We can choose $f(\mathbf{x})$ as we want (unrestricted hypothesis space, no assumed functional form)
- Hence, for a fixed value $\mathbf{x} \in \mathcal{X}$ we can select **any** value c we want to predict. So we construct the **point-wise optimizer**

$$f^*(\mathbf{x}) = \text{argmin}_c \mathbb{E}_{y|x}\left[L(y, c) \mid \mathbf{x} = \mathbf{x}\right] \quad \forall \mathbf{x} \in \mathcal{X}.$$





THEORETICAL AND EMPIRICAL RISK

The risk minimizer is mainly a theoretical tool:

- In practice we need to restrict the hypothesis space $\mathcal{H}$ such that we can efficiently search over it.
- In practice we (usually) do not know $\mathbb{P}_{xy}$. Instead of $\mathcal{R}(f)$, we are optimizing the empirical risk

$$\hat{f}_{\mathcal{H}} = \underset{f \in \mathcal{H}}{\arg\min}\, \mathcal{R}_{\text{emp}}(f) = \underset{f \in \mathcal{H}}{\arg\min} \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right)$$

Note that according to the **law of large numbers** (LLN), the empirical risk converges to the true risk (but beware of overfitting!):

$$\bar{\mathcal{R}}_{\text{emp}}(f) = \frac{1}{n} \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right) \overset{n \to \infty}{\longrightarrow} \mathcal{R}(f).$$

ESTIMATION AND APPROXIMATION ERROR

Goal of learning: Train a model $\hat{f}$ for which the true risk $\mathcal{R}_L\left(\hat{f}\right)$ is close to the Bayes risk $\mathcal{R}_L^*$. In other words, we want the **Bayes regret**

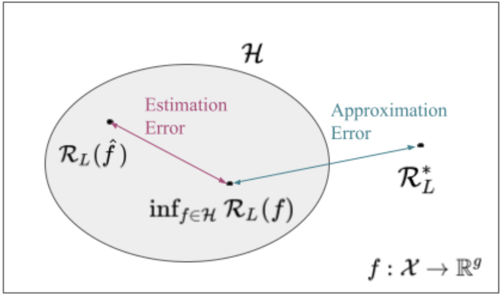
$$\mathcal{R}_L\left(\hat{f}\right) - \mathcal{R}_L^*$$

to be as low as possible.

The Bayes regret can be decomposed as follows:

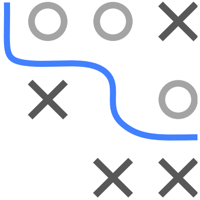
$$\mathcal{R}_L\left(\hat{f}\right) - \mathcal{R}_L^* \quad = \quad \underbrace{\left[\mathcal{R}_L\left(\hat{f}\right) - \inf_{f \in \mathcal{H}} \mathcal{R}_L(f)\right]}_{\text{estimation error}} + \underbrace{\left[\inf_{f \in \mathcal{H}} \mathcal{R}_L(f) - \mathcal{R}_L^*\right]}_{\text{approximation error}}$$

ESTIMATION AND APPROXIMATION ERROR



- $\mathcal{R}_L\left(\hat{f}\right) - \inf_{f \in \mathcal{H}} \mathcal{R}(f)$ is the **estimation error**. We fit $\hat{f}$ via empirical risk minimization and (usually) use approximate optimization, so we usually do not find the optimal $f \in \mathcal{H}$.
- $\inf_{f \in \mathcal{H}} \mathcal{R}_L(f) - \mathcal{R}_L^*$ is the **approximation error**. We need to restrict to a hypothesis space $\mathcal{H}$ which might not even contain the Bayes optimal model f^*.

(UNIVERSALLY) CONSISTENT LEARNERS



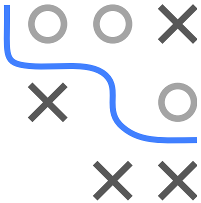
Consistency is an asymptotic property of a learning algorithm, which ensures the algorithm returns **the correct model** when given **unlimited data**.

Let $\mathcal{I}: \mathbb{D} \to \mathcal{H}$ be a learning algorithm that takes a training set $\mathcal{D}_{\text{train}} \sim \mathbb{P}_{xy}$ of size n_{train} and estimates a model $\hat{f}: \mathcal{X} \to \mathbb{R}^g$.

The learning method $\mathcal{I}$ is said to be **consistent** w.r.t. a certain distribution $\mathbb{P}_{xy}$ if the risk of the estimated model $\hat{f}$ converges in probability ("$\overset{p}{\longrightarrow}$") to the Bayes risk $\mathcal{R}^*$ when n_{train} goes to ∞:

$$\mathcal{R}\left(\mathcal{I}\left(\mathcal{D}_{\text{train}}\right)\right) \overset{p}{\longrightarrow} \mathcal{R}_L^* \quad \text{for } n_{\text{train}} \to \infty.$$

(UNIVERSALLY) CONSISTENT LEARNERS



Consistency is defined w.r.t. a particular distribution $\mathbb{P}_{xy}$. But since we usually do not know $\mathbb{P}_{xy}$, consistency does not offer much help to choose an algorithm for a particular task.

More interesting is the stronger concept of **universal consistency**: An algorithm is universally consistent if it is consistent for **any** distribution.

In Stone's famous consistency theorem from 1977, the universal consistency of a weighted average estimator as KNN was proven. Many other ML models have since then been proven to be universally consistent (SVMs, ANNs, etc.).

Note that universal consistency is obviously a desirable property - however, (universal) consistency does not tell us anything about convergence rates ...